

**All-India Institute of Medical Sciences**  
**Ansari Nagar, New Delhi-29.**  
**(RESEARCH SECTION)**

Ref. No.19/Stores/NMR/SSK/2014-15/RS

Dated: 11.02.2015

**Subject:** Purchase of NMR and LC/GC/MS data processing software, for the Department of NMR, at AIIMS, New Delhi-29 on proprietary basis- Inviting comments thereon.

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The request has been received from Dr. S.Senthil Kumaran, Deptt. of NMR, AIIMS to purchase the subject item from M/s Mestrelab Research SL, Spain on proprietary basis. The proposal submitted by M/s Mestrelab Research SL, Spain and PAC certifications are attached.

The above documents are being uploaded for open information to submit objections, comments, if any, from any manufacturer regarding proprietary nature of the equipment/item within issue of 15 days giving reference **No. 19/Stores/NMR/SSK/2014-15/RS**. The comments should be received by office of Stores Officer (RS), Research Section at AIIMS on or before 27/02/2015 upto 12:30 p.m., failing which it will be presumed that any other vendor is having no comment to offer and case will be decided on merits.

**STORES OFFICER (RS)**

**Encl:** Related documents enclosed.

1. PAC Certificate enclosed.
2. Specification of equipment.

**Computer facility:** with request for uploading the same in AIIMS websites for the period of 15 days.

[Contentprovider.aiims@gmail.com](mailto:Contentprovider.aiims@gmail.com)

## Specifications

### *NMR and LC/GC/MS data processing software*

NMR and LC/GC/MS data processing, simulation, prediction and analysis software required with technical support and following specifications:

1. Ability to perform peak picking, integration & multiplet analysis.
  2. Reporting of multiplets in various journal formats (JACS, Angewandte, US Patent).
  3. Intelligent peak pick algorithm. Layout template (complete automation).
  4. Build spectra from multiplet report/peak table
  5. Elementary composition of peaks in  $m/z$  spectrum.
  6. Capability to show mass spectra in profile mode.
  7. Mol Match with several alternatives adducts.
  8. Detection of UV/ visible spectrum in DAD chromatogram.
  9. Prediction of  $^1\text{H}$ ,  $^{13}\text{C}$  & X-nuclei ( $^{15}\text{N}$ ,  $^{17}\text{O}$ ,  $^{19}\text{F}$ ,  $^{29}\text{Si}$ ,  $^{31}\text{P}$ ,  $^{11}\text{B}$ ), also HSQC.
  10. Auto-assignment  $^1\text{H}$  (1D & 2D) &  $^{13}\text{C}$ .
  11. Comparison of predicted with experimental.
  12. Full processing and analysis of 1D & 2D NMR experimental data.
  13. Full processing and analysis of LC/GC MS data (if available).
  14. Generation of theoretical data for the proposed structures.
  15. Comparison of experimental with theoretical data.
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**SOLE MANUFACTURER  
&  
DISTRIBUTOR OF SOFTWARE**

To whom it may concern,

This certifies that Mestrelab Research S.L. is the sole manufacturer and distributor of Mnova NMR, Mnova NMR Lite, NMRPredict Desktop, Mnova MS, Mnova DB, Mnova ASV, Mspin, MestReS, MestReJ and Exsyscalc software.

With best regards,

A handwritten signature in black ink, appearing to read 'J. Cobas'.

Dr. J. Carlos Cobas Gomez  
President

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